Electronic correlations in transport through coupled quantum dots

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The conductance through two quantum dots in series is studied using general qualitative arguments and quantitative slave-boson mean-field theory. It is demonstrated that measurements of the conductance can explore the phase diagram of the two-impurity Anderson model. Competition between the Kondo effect and the inter-dot magnetic exchange leads to a two-plateau structure in the conductance as a function of gate voltage and a two or three peak structure in the conductance vs. inter-dot tunneling.

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The recent observation of the Kondo effect in transport through a quantum dot [1–3] opened a new path for the investigations of strongly correlated electrons. Having confirmed earlier theoretical predictions [4,5], that a quantum dot behaves as a magnetic impurity, these experiments also serve as a critical quantitative test for existing theories. In particular, unlike magnetic impurities in metals which have physical properties determined by the host metal and the impurity atom, the corresponding parameters in the quantum dot case can be varied continuously, enabling, for example, a crossover from the Kondo to the mixed-valence and the empty dot regimes in the same sample [1,2].

The behavior of a lattice of magnetic impurities, such as a heavy-fermion system, is characterized by the competition between the Kondo effect and the magnetic correlations between the impurities. An important step towards the understanding of this problem was taken by Jones and collaborators [6], who studied the two-impurity problem. Their work demonstrated that this competition leads to a second-order phase transition when particle-hole symmetry applies. When this symmetry is broken, this transition is replaced by a crossover [7–9]. In view of the extensive experimental research on transport through two dots in series [10,11], it is thus natural to try and understand how this phase-transition is manifested in the double-dot system, both because such systems may have important applications (such as a quantum-dot laser [12]), and because such a tunable system may reveal detailed information on the corresponding phase diagram.

Transport through a double-dot system (see inset in Fig. 1) has already received much theoretical attention, in particular in the high temperature, Coulomb blockaded regime [12,13]. In experiments the Coulomb charging energy and the excitation energy are much larger than temperature. Accordingly, only a single state on each dot is important, and double occupancy of each dot can be ignored. Denoting the energies of these states by $\epsilon_1 \equiv \epsilon_0 + \Delta\epsilon$ and $\epsilon_2 \equiv \epsilon_0 - \Delta\epsilon$, respectively, and the tunneling amplitude between the dots by t, the isolated double dot system can contain zero, one or two electrons, depending on the chemical potential: $N = 0$ for $\mu < \epsilon_-$, $N = 1$ for $\epsilon_- < \mu < \epsilon_+$, and $N = 2$ for $\mu > \epsilon_+$, with $\epsilon_\pm = \epsilon_0 \pm \sqrt{\Delta\epsilon^2 + t^2}$. In the presence of a finite antiferromagnetic spin-exchange J between the dots, one still has the above three possibilities with ϵ_+ replaced by $\epsilon_+ - 3J/4$ [14]. In the Coulomb blockade regime there will be two peaks in the conductance vs. chemical potential at the degeneracy points $\mu = \epsilon_\pm$. Alternatively, starting from the $N = 2$ regime for $t = 0$, ϵ_+ will increase with increasing t, until it crosses the chemical potential and the ground-state will have a single electron in the double dot system. Again we expect a peak in the conductance at $t = t_+$ corresponding to $\epsilon_+(t_+) = \mu$.

At low temperatures, in addition to a renormalization of the above energy scales, $\epsilon_\pm \to \overline{\epsilon}_\pm$, and $t_+ \to \overline{t_+}$, the Kondo effect starts to play a significant role in the transport. The relevance of the Kondo effect in the double dot system has been studied in [15,16]. Here, we focus on the competition between the Kondo effect and antiferromagnetic exchange, and present detailed predictions for the conductance. (Recently Andrei et al. [17] have investigated a very different realization of this competition, which applies to coupled *metallic islands*, close to points of charge degeneracy – i.e. near the Coulomb-blockade peaks [18]). We find a rich phase diagram leading to interesting features in the conductance as a function of gate voltage and intra-dot tunneling. As the corresponding energy and temperature scales are experimentally accessible, these predictions are relevant to transport experiments in double-dot systems.

To simplify notations, we assume in the following $\epsilon_1 = \epsilon_2 = \epsilon_0$ and $V_L = V_R = V$, where $V_L(V_R)$ is the coupling to the left (right) lead. Then the eigenstates of the double dot system are the even and odd states. As even-odd symmetry is broken anyway by the tunneling t, one can show that the above assumptions have little effect on the underlying physics. Following Ref. [19], the zero-temperature conductance *per spin channel* through the system can be expressed in terms of the retarded

Green functions for the even and odd states $\mathcal{G}^{ret}_{e,o}(\omega)$ as: $g = \frac{e^2}{h}\Gamma^2|\mathcal{G}^{ret}_e(\omega=0) - \mathcal{G}^{ret}_o(\omega=0)|^2$ where $\Gamma \equiv \pi\rho V^2$ and ρ is the density of states in the leads at the Fermi energy. Defining the corresponding *scattering phase-shifts*, $\delta_\alpha \equiv \pi + \arg\mathcal{G}^{ret}_\alpha(\mu)$ (such that δ_α is in the 0-π range), the conductance formula simplifies to

$$g = \frac{e^2}{h}\,\sin^2(\delta_e - \delta_o) \tag{1}$$

The Friedel sum rule relates the total charge *q per spin channel*, on the double dot system, to these phase shifts: $q = (\delta_e + \delta_o)/\pi$. There is, however, no individual relation between δ_α and the occupation of the corresponding state.

For $\mu > \overline{\epsilon}_+$ (or alternatively $t < \overline{t_+}$), there are $N = 2$ electrons in the system ($q = 1$), and states with $N = 0$ or $N = 1$ are high-energy states that can be eliminated from the Hilbert space. The effective low-energy Hamiltonian only involves spin degrees of freedom on the dots. It can be cast into the form of a model of *two Kondo impurities*, with Kondo couplings to the even and odd combinations of the conduction electrons in the leads, an inter-impurity magnetic exchange $J \propto t^2/U$, and a potential scattering term in the leads $V^{e,o}$ such that $V_e - V_o \propto t\,V^2/(\epsilon_0^2 - t^2)$.

Previous studies of the two-impurity Kondo problem (mainly using Wilson numerical renormalization group (NRG)) [6,8] have already yielded information on how the phase shifts δ_e, δ_o behave as a function of the couplings at $T = 0$ in this regime. Let us start with the case $J = 0$. For $t = 0$ there is an even-odd symmetry, and each channel has its own Kondo effect, leading to $\delta_e = \delta_o = \pi/2$, and naturally a zero conductance. As t/Γ is increased, the difference $\delta_e - \delta_o$ increases to reach the value $\pi/4$, at which point the conductance takes its maximum possible value: e^2/h per spin channel. As t/Γ is further increased, the Kondo effect is gradually overcome by potential scattering and one reaches $\delta_o \simeq 0$, $\delta_e \simeq \pi$ in the large t/Γ limit (but still with $t \ll \overline{t_+}$). A slave-boson mean-field theory (SBMFT) presented below (cf. also Ref. [16]) yields in this regime: ($J = 0$, $q \simeq 1$) $\delta \equiv \delta_e - \delta_o = 2\tan^{-1} t/\Gamma$, leading to

$$g = \frac{e^2}{h}\,\frac{4t^2\Gamma^2}{(t^2+\Gamma^2)^2} \tag{2}$$

which reaches its maximum value at $t = \Gamma$ (solid curve in Fig. 1). The Kondo temperature in this regime is of order $T_K = c_1\,T_K^0 e^{c_2 t/\Gamma}$, where the c's are weakly dependent on t/Γ and $T_K^0 \equiv We^{-\pi|\epsilon_0|/\Gamma}$ is the single-dot Kondo temperature. (The SBMFT yields $c_1 = \cos\delta/2$ and $c_2 = \delta/2$). The crucial content of that formula is that the coupled-dot Kondo temperature can be *much larger than the single-dot Kondo temperature* for small J and large t/Γ. This has important consequences for the observability of the effects described in this paper.

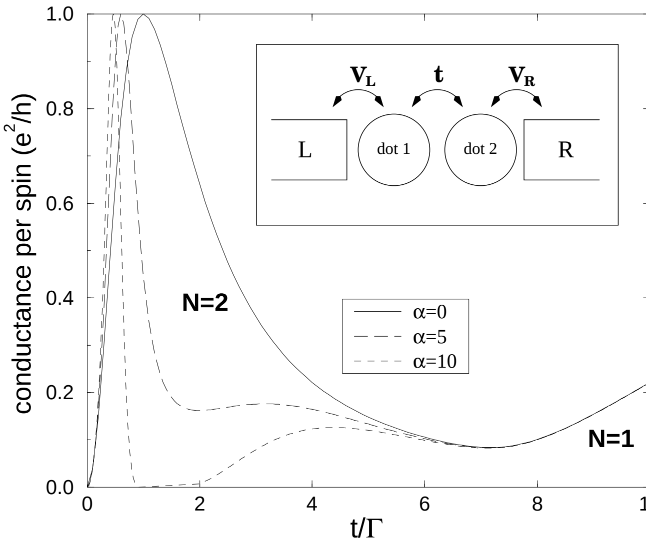

FIG. 1. Plot of the conductance vs. the tunneling between the dots, t, obtained by slave-boson mean-field theory. Due to the Kondo effect in the two-electron regime ($N = 2$) the conductance has a peak at $t = \Gamma$. As t increases beyond $\overline{t_+}$, the Kondo effect is quenched, until the ground-state contains a single electron ($N = 1$), leading to a different Kondo state and an enhanced conductance. For finite antiferromagnetic coupling J (finite $\alpha = \Gamma^2/UT_K^0$), the conductance peak is pushed to smaller values of t and becomes narrower, as the singlet formation destroys the Kondo state. In addition a second maximum in the conductance in the $N = 2$ regime emerges. *Inset*: The double dot system discussed in this paper.

Let us now consider the effect of a finite J. For $t = 0$. the effective two-impurity Kondo model has particle-hole symmetry, and it is known from the work of [6] that a *phase transition* exists at a critical value of the coupling $J_c/T_K^0 \simeq 2.2$. For $J < J_c$, the spin of each dot undergoes a Kondo effect with the leads and $\delta_e = \delta_o = \pi/2$. For $J > J_c$, the two spins are locked into a singlet state and the Kondo effect does not apply, yielding $\delta_o = 0, \delta_e = \pi$. The phase-shift difference δ jumps discontinuously from $\delta = 0$ for $J < J_c$ to $\delta = \pi$ for $J > J_c$. (The conductance is, of course, zero for all J since $t = 0$). Turning on a small value of t/Γ is known to be a "relevant perturbation" on this critical point (with dimension 1/2, identical to that of $J - J_c$) [7,8] and therefore smears the transition into a rapid crossover from $\delta = 0$ to $\delta = \pi$. For J close to J_c, this smearing is described by a crossover scaling function:

$$\frac{\delta}{\pi} = \phi\left(\frac{(J-J_c)/T_K^0}{t/\Gamma}\right) \tag{3}$$

with $\phi(x \to -\infty) = 0$ and $\phi(x \to +\infty) = 1$. As a result, the conductance has a very sharp maximum as t/Γ

is increased for a fixed value of J close to J_c. For J significantly larger than J_c, the conductance remains very small with only a shallow maximum as t/Γ is increased. For intermediate values of t/Γ and J/T_K^0, a quantitative calculation of δ is needed in order to obtain the conductance, using e.g. NRG [6,8,20] or SBMFT. However, much can be said on a semi-quantitative level by using existing knowledge on the two-impurity Kondo problem. The phase shift δ is an increasing function of J, which starts at the value given above Eq.(2), and increases until it saturates at $\delta = \pi$ at a scale J^*. From the above estimate of T_K the ratio J^*/T_K^0 increases exponentially with t/Γ. These considerations, and the knowledge of the crossover around J_c (Eq.(3)), lead to a qualitative contour plot of the conductance in the $(J/T_K^0, t/\Gamma)$ parameter space, throughout the $N \simeq 2$ regime, as displayed in Fig. 2.

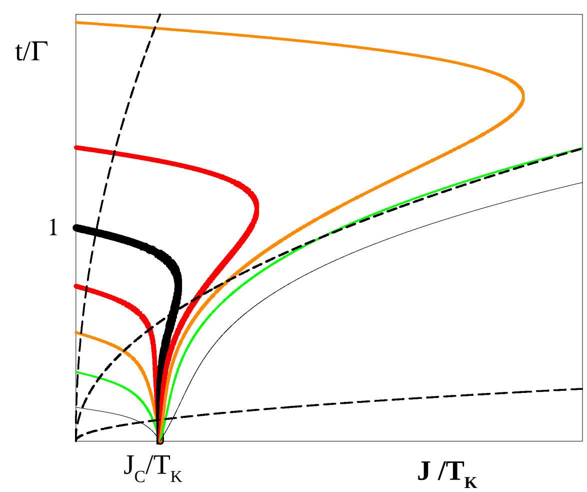

FIG. 2. Schematic contour map of the conductance in the $N \simeq 2$ regime. Thicker lines denote higher conductance, the thickest one corresponding to $g = e^2/h$. The broken lines are three physical contours (for different values of $\alpha \equiv \Gamma^2/UT_K^0$) along which $J \sim t^2/U$.

In practice, the exchange J is not an independent parameter, but is a function of the interdot tunneling, $J \sim t^2/U$. The contour plot above must thus be intersected by a curve $J/T_K^0 = \alpha(t/\Gamma)^2$, with $\alpha \equiv \Gamma^2/UT_K^0$, in order to follow the dependence of the conductance as a function of t/Γ. Since T_K^0 is a very sensitive function of the energy scales (such as ϵ_0 and Γ), the control parameter α can be varied continuously over many orders of magnitude, allowing an experimental investigation of most of the phase-diagram. Thus, as a function of t, the maximum conductance e^2/h is reached for $t \simeq \Gamma$ with a peak width $\Delta t \propto \Gamma$ for small α, while the peak is pushed down to much lower transmission $t \simeq \Gamma/\sqrt{\alpha}$ and becomes very narrow $\Delta t \simeq \Gamma/\alpha$ for large α. In addition, as the saturation scale J^* increases exponentially with t, one may expect, for an intermediate α (middle broken curve in Fig. 2), an additional peak in the conductance vs. t in the $N = 2$ regime. These results are indeed confirmed by the SBMFT calculation (see Fig. 1).

As t is further increased ($t > \overline{t_+}$), the equilibrium charge decreases to $N = 1$ ($q = 1/2$). In this regime the effective Hamiltonian is that of a *single-impurity* Kondo problem in the even parity sector [15], leading to unitary scattering $\delta_e \simeq \pi/2$. In the odd parity sector, we have an almost empty resonant level with $\delta_o \simeq 0$ (Note that $(\delta_e + \delta_o)/\pi = q \simeq 1/2$ consistent with Friedel sum rule). Throughout this regime, we therefore expect the zero-temperature conductance to be maximum $g = e^2/h$ and essentially independent of t. In this regime, the inter-dot exchange J plays little role.

Similar interesting behavior is expected as a function of gate voltage, that controls the depth of the level energy ϵ_0 with respect to the chemical potential (see Fig. 3). For a very deep level the Kondo temperature is exponentially small, and thus $J/T_K^{(0)}$ is large and quenches the Kondo effect. As ϵ_0 increases, the Kondo temperature increases and we enter the ($N = 2$) Kondo state, and a finite conductance. This conductance remains constant (at zero temperature) at a value *smaller than* e^2/h, determined by the value of t, until ϵ_0 crosses the Fermi energy and a new ($N = 1$) Kondo state is formed. There the conductance is given by its maximum value, e^2/h per spin. As ϵ_0 is further increased the double dot system becomes empty and the conductance drops to zero.

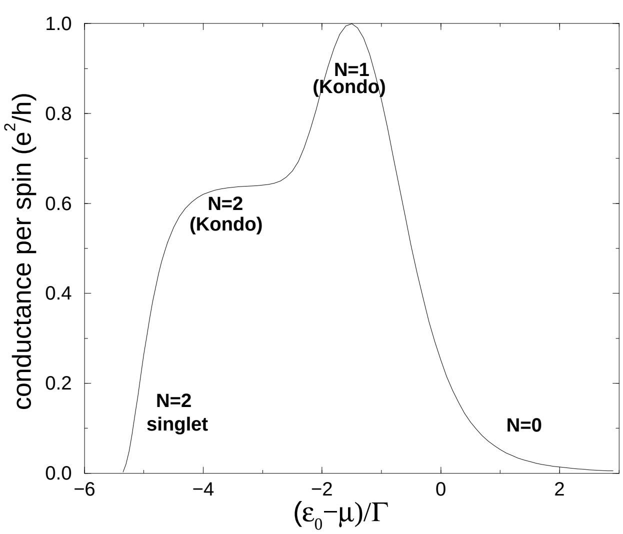

FIG. 3. Plot of the conductance vs. the level energy, as obtained from SBMFT (for $t = 2$ and $U/\Gamma = 10^4$). The conductance rises from a very small value (the singlet regime, $J \gg T_K$), to a t-dependent value ($N = 2$ Kondo regime, $J \ll T_K$), and then to $g = e^2/h$ ($N = 1$ Kondo regime) before dropping to zero for an empty dot.

To substantiate these semi-quantitative arguments we have performed a quantitative calculation of the phase shifts and the conductance using a slave-boson mean-field approximation. This method becomes exact as the number of spin-degrees of freedom goes to infinity, and has been previously used in order to study the two-impurity Anderson model in Ref. [7]. It was recently applied in the present context in Ref. [16] but only in the case $J = 0$. We have solved numerically the full set of equations including the tunneling t and exchange J, but we only quote here the simplified version of the equations [7] that hold in the $q = 1$ regime (one electron in the double dot system per spin-state, corresponding to $N = 2$). For small enough values of J/T_K^0, the phase-shift difference δ is given by the solution of:

$$\frac{2\pi}{\delta} e^{\delta t/2\Gamma} \left(\sin\frac{\delta}{2} - \frac{t}{\Gamma} \cos\frac{\delta}{2} \right) = \frac{J}{T_K^0} \qquad (4)$$

As J is increased beyond a critical coupling J_c^{SB}, δ reaches the value π: this is either a smooth transition for $t > 1/\pi$, or a first-order jump for $t < 1/\pi$ (determined by free-energy considerations). The existence of a phase transition even for non-zero values of t/Γ is an artifact of the SBMFT approximation: J_c^{SB} should actually be interpreted as an estimate of the saturation scale J^* discussed above. This spurious transition does not affect qualitatively the behavior of the conductance, except when it becomes very small: there a strictly zero-value of g can be found (as evident on Fig. 1) whereas the real system would have only a very small but finite g. The SBMFT also provides a quantitative estimate of the Kondo scale for the coupled dot system in the $q \simeq 1$ regime, as mentioned after Eq. (2).

In conclusion, we have demonstrated that measurements of the conductance through a double-dot system can explore the phase diagram of the two-impurity Anderson model. By changing the control parameter $\alpha = \Gamma^2/UT_K^0$ (which depends sensitively on gate-voltage), one can make various cuts through the phase-diagram (Fig. 2), leading to non-trivial features in the conductance vs. gate-voltage and inter-dot tunneling (Figs. 1 and 3). As the relevant temperature scale can be much higher than the single-dot Kondo temperature we believe that these predictions could be tested experimentally.

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